Butyl nitrate
928-45-0 | DTXSID70239143

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 132 °C

Global applicability domain: Inside

Local applicability domain index: 8.75e-01

Confidence level: 8.75e-01

Nearest Neighbors from the Training Set

Image not found
Butyl nitrate
Measured: 133
Predicted: 132

Image not found
Isobutyl nitrate
Measured: 123
Predicted: 126

Image not found
Isoamyl nitrate
Measured: 146
Predicted: 143

Image not found
Isoamyl nitrate
Measured: 146
Predicted: 143

Image not found
Amyl nitrate
Measured: 157
Predicted: 151